FUEL DEPLETION ANALYSES FOR THE HEU CORE OF GHARR-1; Part I: ACTINIDE INVENTORY

S. Anim-Sampong[1], E.H. K. Akaho,[1] H. O. Boadu[1], J.D.K. Intsiful[2], S. Osae[3]

Dept. of Nuclear Eng. & Mat. Sci., NNRI,
[2]National Centre for Mathematical Sciences, [3]Dept. of Physics, NNRI,
Ghana Atomic Energy Commission
P.O. Box LG 80, Legon, Accra. Ghana

ABSTRACT
The Ghana Research Rreactor-1 (GHARR-1), a 30kW, 90.2% HEU fueled (U-Al) MNSR type reactor went critical on December 17, 1994. Under operating conditions of 2.5hours per day for five days a week at a peak thermal neutron flux of $1.0x10^{12}n/cm^2.s$, the estimated core life is ten years. After the fuel is depleted, the entire spent fuel assembly will be replaced with a fresh LEU core in the spirit of the RERTR program and in accordance with current trend. This paper presents the results of multigroup fuel burnup and depletion analysis of the GHARR-1 fuel lattice using the WIMSD/4 transport lattice code. The results contained in this paper would be used as microscopic database in performing criticality safety analysis and shielding calculations for the design of a spent fuel storage cask for the GHARR-1 core.

Introduction

During the operating lifetime of a nuclear reactor, i.e., from the beginning of life (BOL) to end of life (EOL), the isotopic inventory of the nuclear fuel is in a state of continuous evolution. This is the result of fuel depletion or burnup due to nuclear reactions [1]. For GHARR-1, burnup calculations are necessary for the prediction of long- term changes in the isotopic composition of its highly enriched uranium (HEU) fuel due to exposure or irradiation by neutrons during its operation. These changes, e.g., core power distributions, flux spectrum variations, power peaking factors and fraction of reactor power per fuel lattice zone of the core assembly, which occur in space and time, strongly influence the operating life, stability and control of the reactor. In particular, it is important that there is enough excess reactivity to operate the reactor from the time of fresh fuel loading to the desired final exposure or shutdown of the reactor.

Lattice burnup calculations in thermal reactors are complicated by the necessity for the use of transport theory to represent fuel rods, rod clusters, control rods and burnable absorbers, by many time-dependent variables which must be considered in the analyses, and by geometric complexity which introduces time-dependent, spatial-spectral variation [2]. Transport codes are therefore needed to perform reactor lattice burnup calculations. The WIMS code (versions D/4 and 5B) is an example of such codes and are presently being used in Ghana by the Reactor Physics Research Group of the Ghana Atomic Energy Commission.

In this work, multigroup local burnup calculations have been performed on a 5-region lattice cell of the 90.2% HEU GHARR-1 fuel assembly using the WIMSD/4 transport code. The aim of this paper is to present the results of the lattice depletion analysis of the fuel, paying particular attention to the energy and burnup variations of the flux spectrum, cell multiplication factors, and the neutron cross sections. The burnup-dependent cross sections would be used as input data for 3-D global reactor diffusion calculation to study the fuel depletion at the global level.

Reactor Description

The active region of the GHARR-1 core is a very small fuel assembly. Its active height and effective diameter are 23 cm and 23 cm respectively. It consists of a central control rod guide tube surrounded by ten concentric rings of fuel lattices containing three hundred and forty-four fuel elements, four tie and six dummy rods located respectively in the 8-th and 10-th lattices in the top and bottom grid plates. The average radial pitch between any two consecutive fuel rings or lattices is 10.95mm. [3]. A schematic diagram describing the lattice configuration of the core is shown in Fig. 1[4]. Presently, the core is reflected at the bottom and radially with beryllium alloy material.

Outline of the Burnup Calculation

Burnup calculations involve some approximations. One such approximation is the decoupling of coupled effects. These are microscopic-macroscopic decoupling as well as space-time decoupling. The former suggests that burnup calculations, in practice, are performed at two levels [2, 5-8].

1. ***Microscopic level***: In lattice burnup calculations, the neutron spectrum and fuel element geometry are represented in detail and involves the accurate computation of the fuel element reaction rates and fuel composition (uranium depletion and plutonium build-up) as functions of burnup in a lattice cell representative of a given region of the core using a transport lattice code. The microscopic calculations re used to provide homogenized parameters such as neutron cross sections as functions of burnup which serve as input data for overall global reactor analyses

2. ***Macroscopic level:*** This level concerns the determination of global depletion behavior of the reactor core. This includes the long term behavior of reactivity variations, core power distribution, core burnup and the total core fuel material inventories.

Fuel depletion analysis is concerned with the prediction of long term changes in the isotopic composition of reactor fuel caused by the exposure to neutrons of varying flux levels leading to fuel irradiation in the core of a reactor during operation. These changes in isotopic composition, witnessed in both time and space dimensions have important effects on the operating life of the reactor, its stability and control and reactor economics as a whole. Thus in a depletion study, the following quantities and operational parameters must be monitored:

> fuel isotopic composition which involves the consumption of fissile(e.g. U^{235}) nuclides, conversion of fertile isotopes(e.g., U^{238}) and the production of fission products and other burnable fission product poisons(Xe^{135}, Sm^{149}, B^{10}, etc),
>
> core reactivity balance by determining the change in excess reactivity over a period of core operation and then adjusting control elements to compensate for loss of reactivity.

In space-time decoupling, the time dependence of the fuel burnup and changes in the neutron flux distribution are conveniently handled by separating the depletion and neutronic calculations. In depletion calculations, the reaction rates equations are solved and spatial effects are ignored.

During neutronic calculations, time effects are ignored and the static multigroup neutron diffusion equation is solved [9].

3.0. Review of WIMSD/4 Lattice Burnup and Depletion Calculations: Theory

In this section, a review of local burnup calculations as outlined in the WIMS literature is presented. Particular reference is made to the presentations of Roth [10]), Halsall [11-13], Taubman [13] and Kulikowska [14].

In the WIMSD/4 transport lattice code, the fuel burnup calculations constitute the last step of the program chain. The WIMS calculational and burnup computational flowcharts are shown respectively in Figs.2 and 3 [10-12,14]. The multigroup neutron fluxes, ϕ_{igl} (g=group index, l = spectrum type) are read for a representative cell of the lattice and condensed into a fewgroup energy structure. They are then used to calculate effective microscopic cross sections in a fewgroup scheme on which resonance corrections are imposed as shown in Fig. 3. The fewroup fluxes $\Phi_{G,z}$ (G= fewgroup index , z=zone index, m=material index) are calculated in the main transport routine and averaged over the cell material volumes by the formula

$$\Phi_{G,z}^{T} = \frac{\sum_{m\in z}\left(\Phi_{G,m}^{T} V_{z(m)}\right)}{\sum_{m\in z} V_{z(m)}} \qquad (1)$$

where Φ^T is the flux computed in the main transport routine.

The burnup calculations are performed in Chain. These include:

1. Preparation of tables of effective microscopic absorption and fission cross sections in few energy groups for the various nuclides of each burnable material in the cell using information such as microscopic cross sections data library of the lattice code and resonance data and neutron fluxes from the spectrum calculation. Preparation of multigroup macroscopic crosses sections for absorption and fission reactions and corrected for modifications in the isotopic number densities due to burnup. These macroscopic cross sections are calculated in each short step using the number densities:

$$\Sigma_{G}^{x} = \frac{\sum_{z}\left\{V_z \Phi_{G,z}^{n-1} \sum_{i,m\in z}\left(N_{i,m}\sigma_{G,i,m}^{x}\right)\right\}}{\sum_{z} V_z \Phi_{G,z}^{n-1}} \qquad (2)$$

where *x is* the reaction type(absorption or production and *n* is the number of current burnup short step. The flux corresponding to the n-th burnup step assumes the values

$$\Phi_{G,z}^{n-1} = \begin{cases} \Phi_{G,z}^{T}, n = 1 \\ \Theta_{G,z}^{n-1}, n \rangle 1 \end{cases}$$

The total neutron flux is calculated according to Eq.(3)

$$\Phi_G^c = \frac{\sum_z V_z \Phi_{G,z}^{n-1}}{V_c \Phi_G^c} = \frac{\sum_z V_z \Phi_{G,z}^{n-1}}{V_c} \qquad (3)$$

where $V_c = \sum_z V_z$ determines the total volume.

2. A POISON option is available in the burnup routine which provides additional solution of the neutron transport equation by collision probability method for a subsystem consisting of a number of regions as defined by the POISON card

3. Solution of the fewgroup criticality equation for the homogenized lattice cell with cross sections calculated in (1) for absorption and production reactions and taken from the main transport (scattering) are solved at each short burnup stage using the diffusion equation

$$\left\{\Sigma_G^a + D_G B^2 + \sum_{h\neq G}\Sigma^{Gh}\right\}\Phi_G^n + \lambda\left\{\Sigma_G^{a'} + D_G B^{2'}\right\}\Phi_G^n$$

$$= \sum_{h\neq G}\left(\Sigma^{hG}\Phi_h^n\right) + \left(\rho + \lambda + \rho'\right)\chi_G \sum_h \left(\nu_h \Sigma_h^f \Phi_h^n\right) \qquad (4)$$

where the unprimed quantities are constant coefficients of the equation while those with primes denote control quantities. Soluble poison control is described by the quantity $\Sigma_G^{a'}$ while $B^{2'}$ defines the geometrical buckling parameter. The eigenvalue λ is calculated in the presence of the 3rd and 4th entries on the input data card ***BUCKLING*** in the main transport routine section. In matrix form, Eq.(4) becomes

$$(\mathbf{A}+\lambda\mathbf{B})\Phi^n = (\rho+\lambda\rho')\chi(\mathbf{F}\Phi^n) \qquad (5)$$

where **A** consists of absorption, leakage and scattering
B defines the term modifying the neutron balance for k_{eff}=1
χ is the fission spectrum
F.Φ^n is a fission source which can be normalized to an arbitrary value.

In a criticality search for k_{eff}, matrix **B** equal zero and the reactivity variables are defined such that

ρ=1 ρ'=0 for buckling search

ρ=0 ρ'=1 for k_{eff} computation

Generally, the control search is available only for the buckling and it is a standard option in burnup calculations by many code users. For k_{eff} search in the n-th burnup step, the matrix equation (Eq.5) assumes the form:

$$\mathbf{A}.\Phi^n = \lambda.\chi.\mathbf{F}.\Phi^n \qquad (6)$$

Assuming the normalization; $\mathbf{F}.\Phi^n = [\mathbf{E}]$, where **[E]** is a unit matrix, we obtain

$$\mathbf{A}.\Phi^n = \lambda.\chi, \qquad \Phi^n = \lambda.\ \mathbf{A}^{-1}.\chi$$

Defining $\mathbf{A}^{-1}.\chi = \Psi^n$ and multiplying both sides by **F** gives

$$1 = \lambda.(\mathbf{F}.\ \Psi^n), \qquad k_{eff}^n = \mathbf{F}.\ \Psi^n$$

The macroscopic fission cross sections are then computed and printed for all materials undergoing burnup and for the entire cell together with the few and two-groups fluxes according to:

$$\Sigma_{m,G}^n = V_{z\in m}\phi_{G,z\in m}^n \sum_{i=1}^{NNF}\left(N_{im}\sigma_{Gim}\right) \qquad (7)$$

The cell quantities are also calculated through summation over zones, *z*, and the two-group values over the respective groups. The fluxes are integrated over the cell volume. The fission products (***FP***) are also computed according the formula

$$FP = \sum_{G,z,m}\left\{\sum_i\left(N_{im}\sigma_{Gim}Y_i\right)\right\} \qquad (8)$$

4. The flux normalization to a required power (or flux) level and calculation of reaction rates for absorption, fission and capture reactions for each burnable nuclide in each cell material are made. The fission rate (***FR*)** is calculated as

$$FR = \sum_i\left\{\sum_m\left[V_{z(m)}N_{im}\sum_G\left(\sigma_{iGm}^f\phi_{G,z(m)}^n\right)\right]_i\right\}f^{n-1} \qquad (9)$$

where f^{n-1} is a normalization factor taken from the previous short step and is defined as the mean energy per fission. In troduced into the WIMSD/4 code by Aragonnes and Ahnert, the mean fission energy (***E***) measured in units of MeV/fission is calculated as

$$E = \frac{\sum_i\left\{\varepsilon_i\sum_m\left[V_{z(m)}N_{im}\sum_G\left(\sigma_{Gim}^f\phi_{G,z(m)}^n\right)\right]\right\}}{0.6025x1.6x10^{-19}FR} \qquad (10)$$

where ε_l is the energy release per fission for isotope *i*. The isotopic content of fissionable material in the fresh fuel is defined in the WIMS code as the number of grams of fissionable isotopes in 1cm height of the lattice cell (unit or cluster) multiplied by Avogadro's constant. Mathematically, this quantity can be calculated for isotope *i* at the first entry into the code according to the formula

$$a = \sum_m\left\{V_{z(m)}\sum_i\left[N_iA_i\right]\right\} \qquad (11)$$

where *i* - isotope index and A_i is the atomic number of isotope *i* read from the WIMS data library. In particular, *a* is used in computing the flux level for which purpose the power in the n-th burnup step, P^n, is calculated on the basis of actual number densities N_{im}, and the neutron fluxes $\phi^n_{G,z(m)}$ as

$$P^n = \frac{\sum_i \left\{ {}_iY_i \sum_m \left[V_{z(m)} N_{im} \sum_G \left(\sigma^f_{iGm} \phi^n_{G,z(m)} \right) \right] \right\}}{a} \qquad (12)$$

The normalization factor, *f,* introduced in Eq (9) can then be obtained as the ratio

$$f^n = \frac{P^0}{P^n}$$

The normalization factor is used in the next burnup stage to normalize the neutron flux defined in Eq (9) and also for re-normalizing the neutron flux in the different energy groups and the material zones, as well as the reaction rates.

5. The last step in the WIMS burnup calculation involves the performance of trapezoidal integration of the burnup equations to obtain new isotopic number densities for each burnable material *m* and nuclide *i*, with the burnup equation expressed in the form:

$$\frac{dN_i(t)}{dt} = -\lambda_i N_i(t) - A_i N_i(t) + \sum_k \delta(i, j_1(k)) \alpha_{ki} C_k N_k(t)$$

$$+ \sum_k \delta(i, j_2(k)) \beta_{ki} \lambda_k N_k(t) + \sum_k \gamma_{ki} F_k N_k(t) \qquad (13)$$

where N_i = the number density of nuclide *i*
λ_I = decay constant for nuclide *i,*
A_I = absorption reaction rate for nuclide *i*
F_I = fission reaction rates
C_I = capture reaction rates calculated in step (4*)*
γ_{ki} = yield of fission product *i* computed from the fission of nuclide *k*
α_{ki}, β_{ki} = product fractions of isotope *k (*equal to 1 for nuclide *k* with single capture or decay product*)*
$j_1(k)$, $j_2(k)$ = *identifiers of all products from isotope k and the delta functions* $\delta(i,j)$ indicate that the contribution occurs when *i=j.*

The first and second terms of the balance equation (Eq.13) describe losses by radio-active decay of isotope *i*, and neutron capture respectively. The third, fourth and fifth terms represents gains due to neutron transmutation of nuclide *k* to nuclide *i,* decay of nuclide *k* to *i* and production of nuclide *i* through fission product formation respectively. Eq.13 can be written compactly in the form

$$\frac{dN_i(t)}{dt} = -(\lambda + A_i)N_i(t) + \sum_k q'_{i,k}(t)N_k(t) = \sum_k q_{ik}(t)N_k(t) \qquad (14)$$

where

q_{ik}, are the production terms calculated from yields of fission products *i* from fission of nuclide *k,* production fractions, capture and fission reaction rates.

In particular, if $\lambda_l > \lambda_0$, the assumption $dN_i/dt=0$ is made and Eq.(13) reduces to

$$N_i(t+\delta t) = N_i(t) + \frac{\sum_k q_{ik}(t)N_i(t)}{\lambda + A_i} \qquad (15)$$

Finally, the isotopic weight contents are calculated after the last burnup step, by the formula

$$W_{im} = \frac{10^{24}\pi}{N_A}\sum_z N_{im}V_{z(m0}A_i \qquad (16)$$

where W_{im} – defined in grams per 1cm of cell height
N_a – Avogadro's number and A_i is as defined before.

The microscopic cross sections are taken from the data library and the resonance effects from the first step of the burnup calculation.

4.0. Method of Analysis

Calculation of thermal reactor lattice depletion in Ghana are presently, based upon the lattice codes of the WIMS family [15], namely the WIMSD/4 and just recently the WIMSD5B versions. The codes perform general 1-D depletion calculations by means of information on the consequences of capture, decay or fission for each nuclide stored in its 69-energy group data library [5].

In this work, instructions for the preparation of standard input data for lattice burnup calculations and depletion analyses as outlined in the WIMSD/4 lattice code [11, 16] were followed. A 5-region pin cell lattice model based on an earlier work [4], comprising fuel, clad, coolant, dummy and structure material regions (Fig. 4) was used. As required, the plutonium isotope, Pu^{239}, was included as a trace in the isotopic compositions of the burnable material (fuel). A 4-energy group was used in performing the multigroup transport calculations. In particular, the discrete ordinate spatial model (DSN) which solves the differential form of the transport equation by the Carlson-S_N (N=4) approach was adopted for the solution of the Boltzmann multigroup neutron transport equation.

The residence time t_r and the specific power P_s, sometimes called power rating are data parameters required for specification on the ***POWERC*** card. It is calculated according to the formula:

$$P_s = \frac{10^3 P}{n_f g_u} \tag{17}$$

where

P = reactor thermal power (kW)
n_f = total number of fuel elements in the core
g_u = total uranium loading in the fuel (U^{235}+U^{238}) in grams

According to Zhou [17], the amount, in grams of U^{235} [$g_{U\text{-}235}$] in a fuel element is calculated using the relationship:

$$g_{U-235} = \rho_f V[1-p]Xf_m \tag{18}$$

where ρ_f = density of fuel
p = volume porosity (%)
V = volume of fuel
X = weight fraction of uranium in the fuel

The factor f_m, is defined according to the formula:

$$f_m = \frac{m_{U-235}\varepsilon}{m_{U-235}\varepsilon + m_{U-238}(1-\varepsilon)} \tag{4.3}$$

where ε is the enrichment factor, and $m_{U\text{-}235}$, $m_{U\text{-}238}$ are the atomic masses of U^{235} and U^{238} respectively. The volume of the cylindrically configured fuel element corresponding to an active height h and outer diameter d_o is also expressed as

$$V\left(\frac{\pi d_o^2}{4}\right)h \tag{19}$$

The fuel density is calculated using the expression

$$\rho_f = \frac{3.3596(1-p)}{1.2443 - X} \tag{19}$$

In the design specifications for GHARR-1, the critical mass of U^{235} for the 90.2% HEU fuel is 2.88 g out 3.169 g of total uranium per fuel element. This is corresponds to a maximum value of 1% for the core. The residence time is then determined using the formula

$$t_r = \frac{\left(B/n_s\right)}{P_s} \tag{20}$$

where B is the specific burnup and n_s is the number of burnup steps. Neutronic design calculations of the core [17], indicate that the maximum burnup is 1%. This core burnup is generally required for computation of the residence time. The core was then depleted from 0 to 10000 MWd/tU in n_s.

5.0. Results and Discussion

The results of WIMSD/4 lattice burnup and isotopic fuel depletion analysis for the 5-region lattice cell of the GHARR-1 fuel assembly are shown in Figs 5 – 11. The variations of the lattice k-infinity and flux spectrum calculations as functions of fuel burnup are illustrated in Fig. 5. The trend is as expected [18] and consistent with the literature [19]. With burnup, nuclear fuel is depleted and the changes in the isotopic composition could have an influence on the neutron spectrum. The effects on the GHARR-1 fuel can be seen in Figs. 6-8, where the isotopic depletion of U^{235} and U^{238}, as well as the build-up of U^{236}, Pu^{239}, Pu^{240}, and Pu^{241} are demonstrated through the variation of their atom number densities with burnup. Similar burnup characteristics for the isotopic ingredients and weight percents for these actinides are shown in Figs 7 and 8 respectively. These results show a decreasing (consumption) trend for U^{235} and U^{238} as the fuel is depleted. On the contrary, an increasing or build-up behavior is observed for the other actinides. However, the build-up of Pu^{239} is quite insignificant. Figs.9-11 show the WIMSD/4 plots of the diffusion coefficient, macroscopic absorption and ν*fission cross sections with burnup. The plots show that the neutron cross sections do not vary much within the 1% burnup range for the GHARR-1 HEU fuel

6.0. CONCLUSION

The WIMSD/4 transport physics lattice code has been used to perform multigroup lattice cell depletion analysis on the 90.2% HEU fuel of the GHARR-1 fuel assembly. The following conclusions can be drawn based upon the present analysis:

1. There are no significant differences in the neutron spectrum for different burnup values. The neutron cross sections are therefore not expected to vary much within the burnup range.

2. The trend of variations of the isotopic compositions of the various nuclides in the fuel are consistent with earlier work.

3. No significant quantities of Pu^{239} are produced in the spent fuel during depletion to attract any fears for nuclear weaponry.

For further work, there is a need to validate the current results with other depletion codes such as ***FISSPROD*** and the multipurpose code ***SCALE*** developed at the Oak Ridge National Laboratory. The results of the lattice burnup and isotopic depletion analysis would be used to perform 3-D global core depletion studies. Criticality safety analysis and shielding calculations would then performed using the SCALE code to design a storage cask for the GHARR-1 spent fuel.

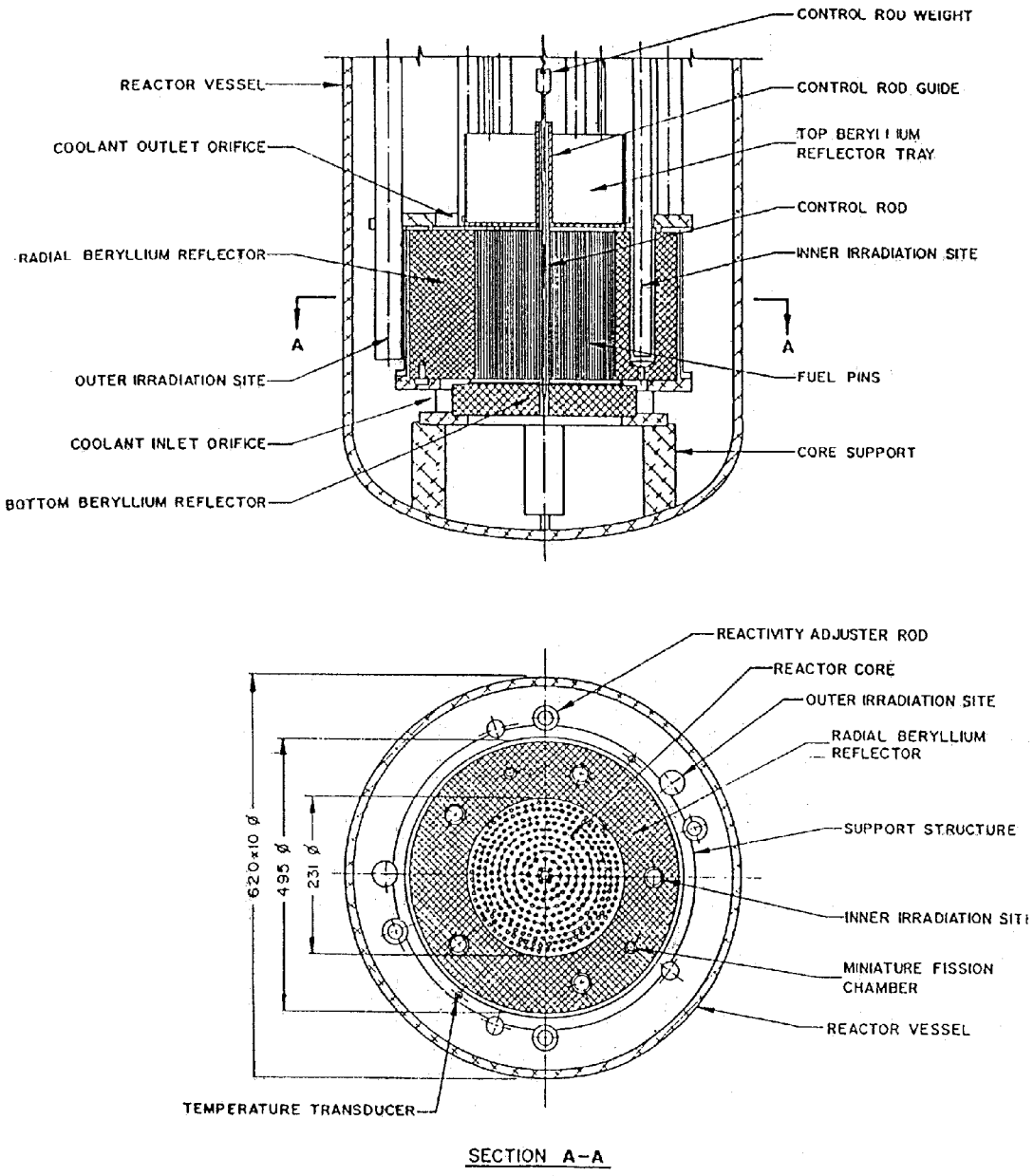


Fig. 1. Cross sectional view through reactor core

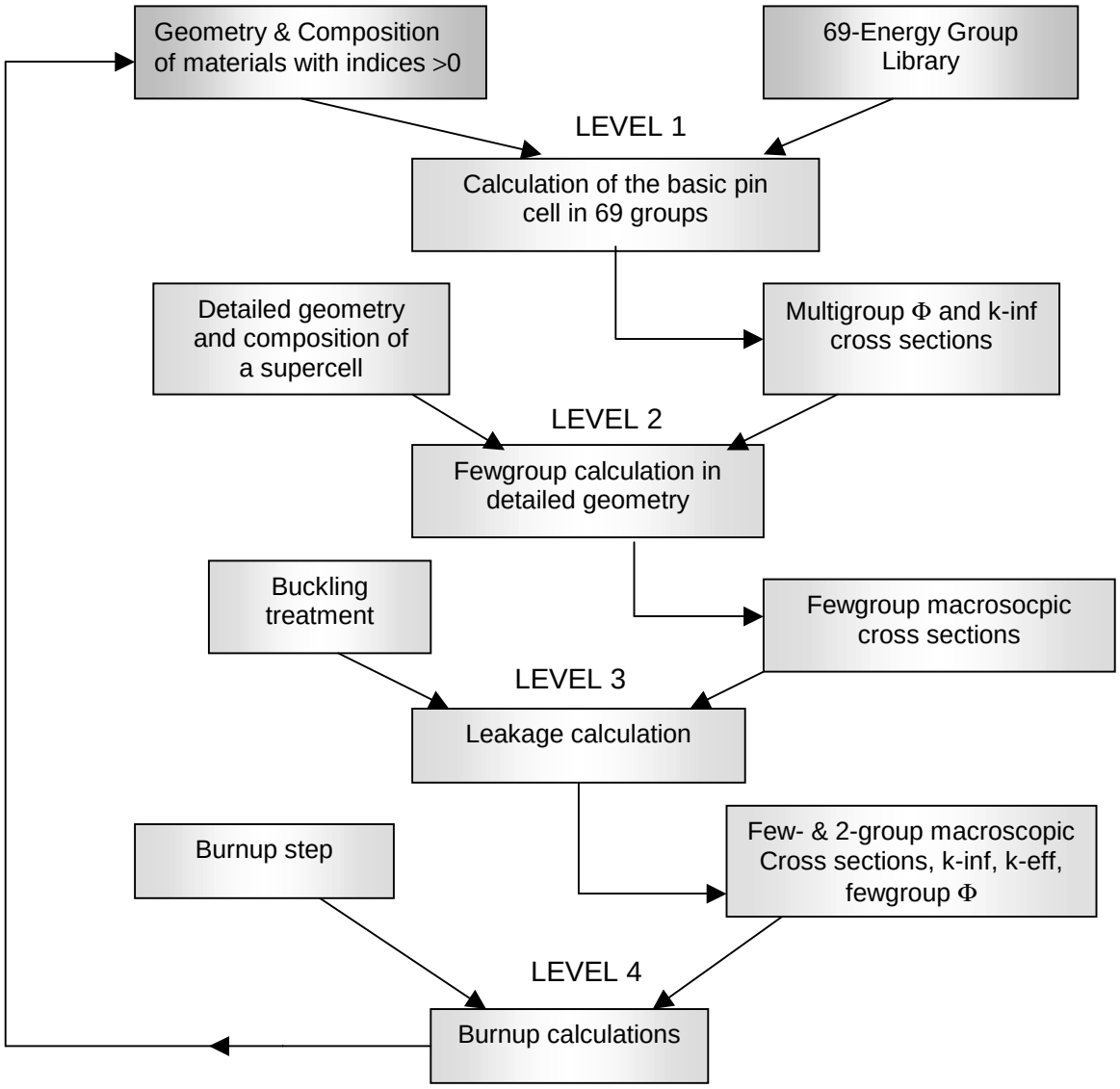


Fig. 2: Simplified flowchart of WIMS calculations

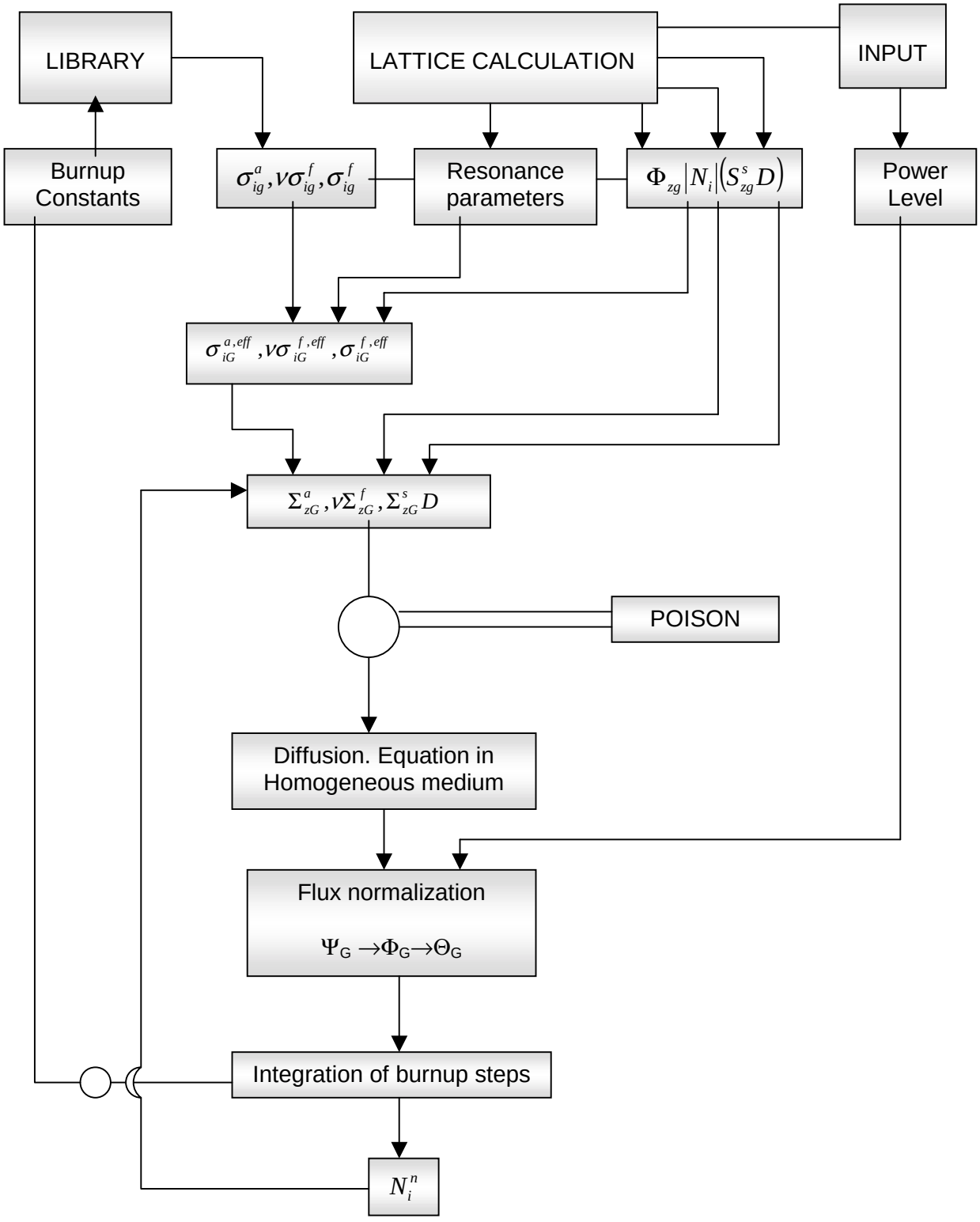


Fig. 3: Flowchart of WIMSD Burnup calculations

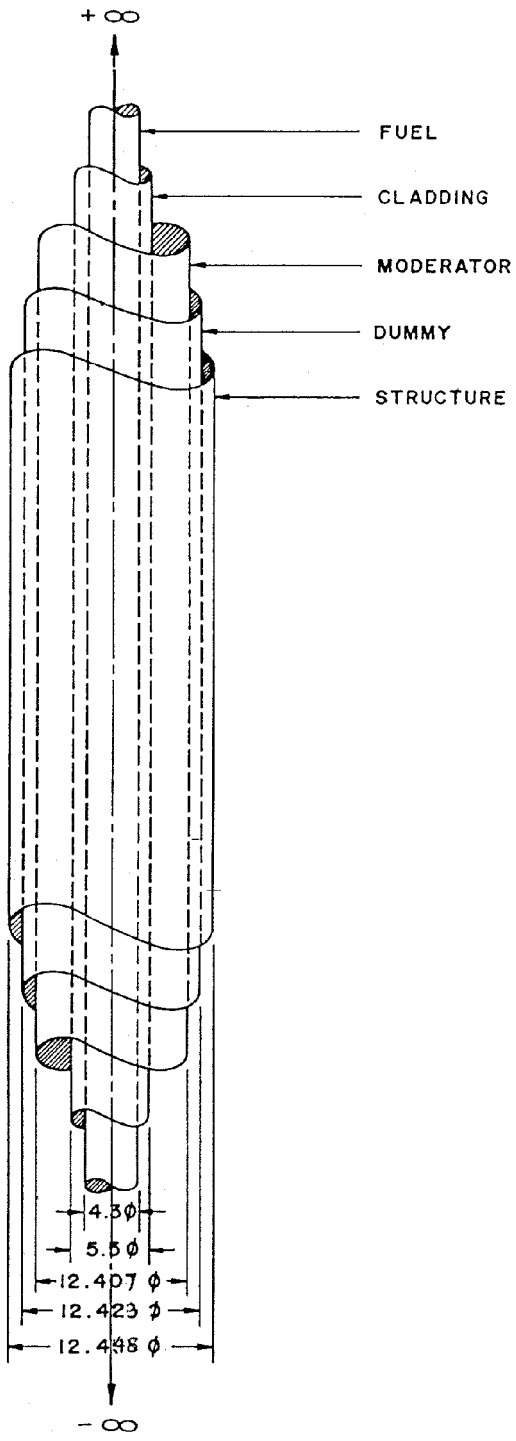


Fig. 4 Fuel Lattice Cell

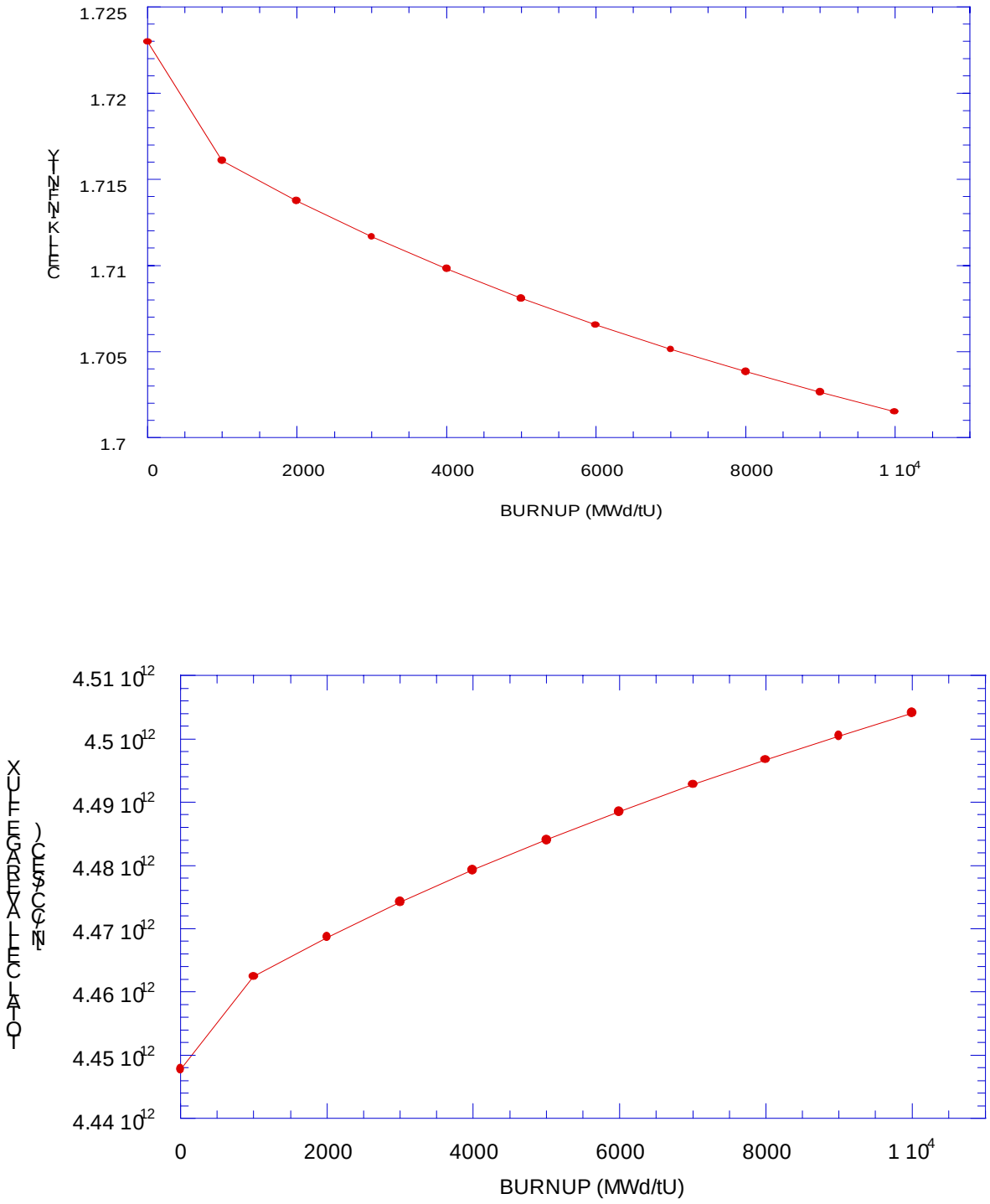


Fig. 5: Variation of Cell k-infinity and Flux Spectrum with Fuel Burnup

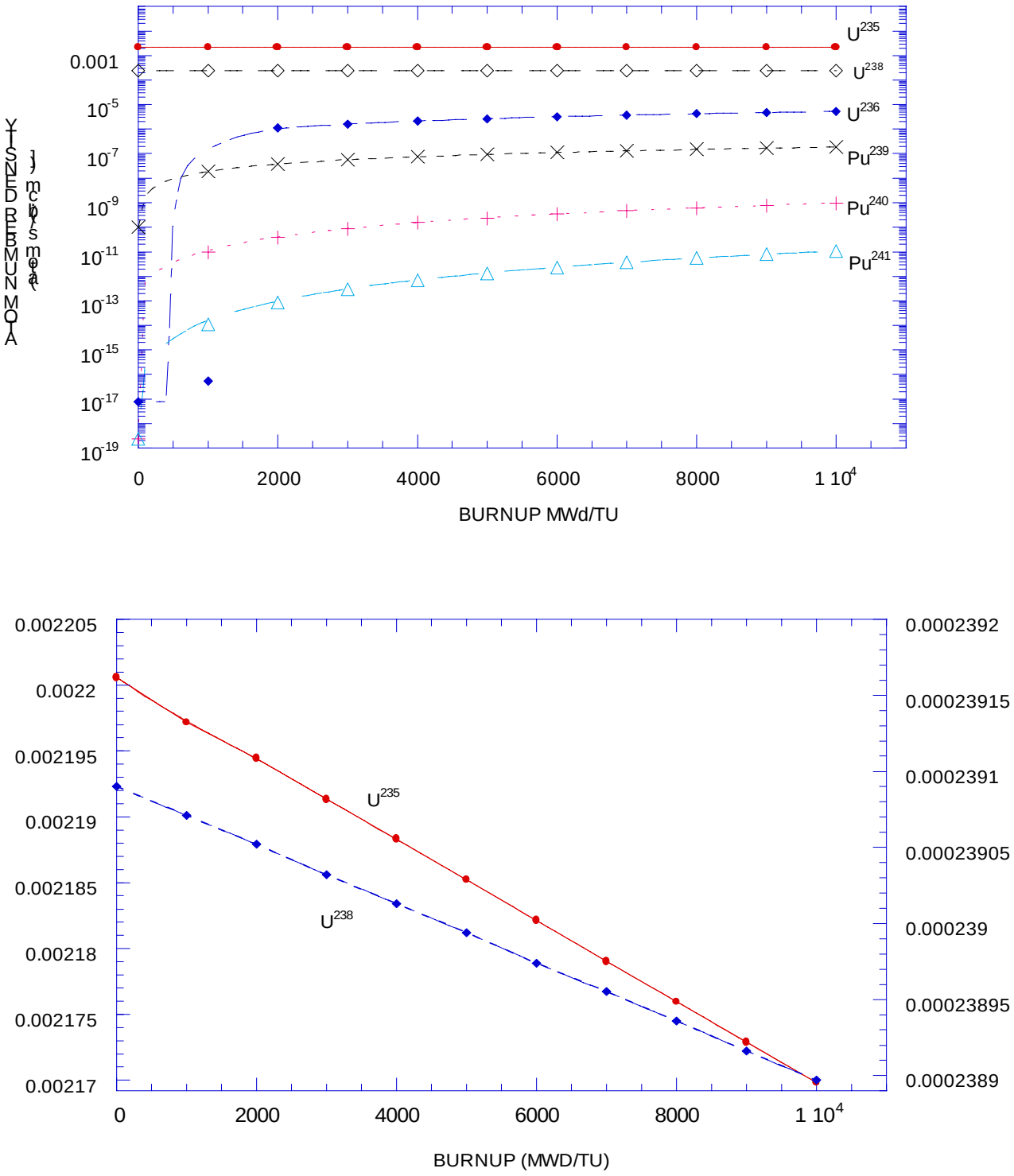


Fig. 6: Actinide Inventory: Atom Number Density vrs. Fuel Burnup

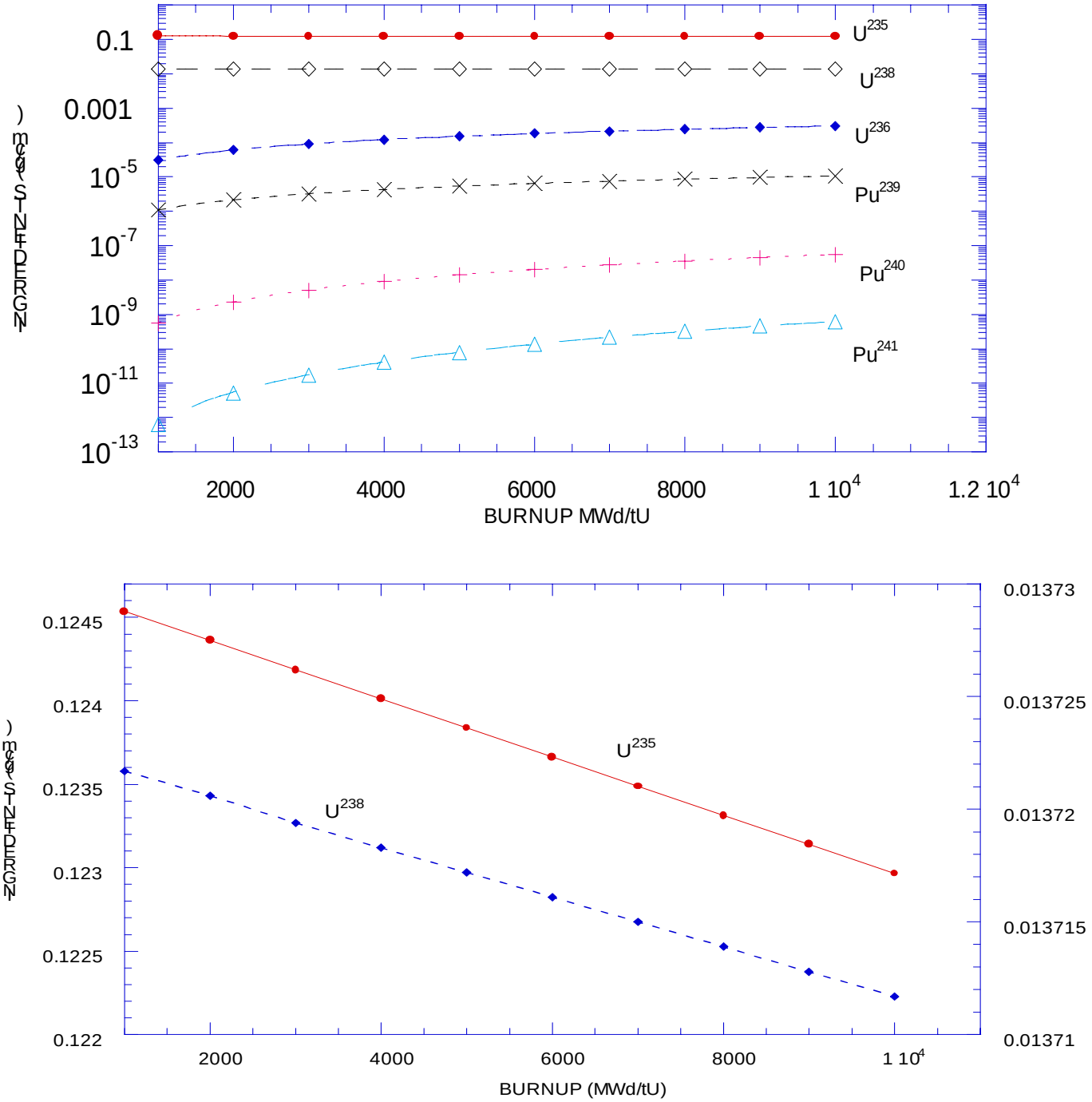


Fig. 7: Actinide Inventory: Ingredients vrs. Fuel Burnup

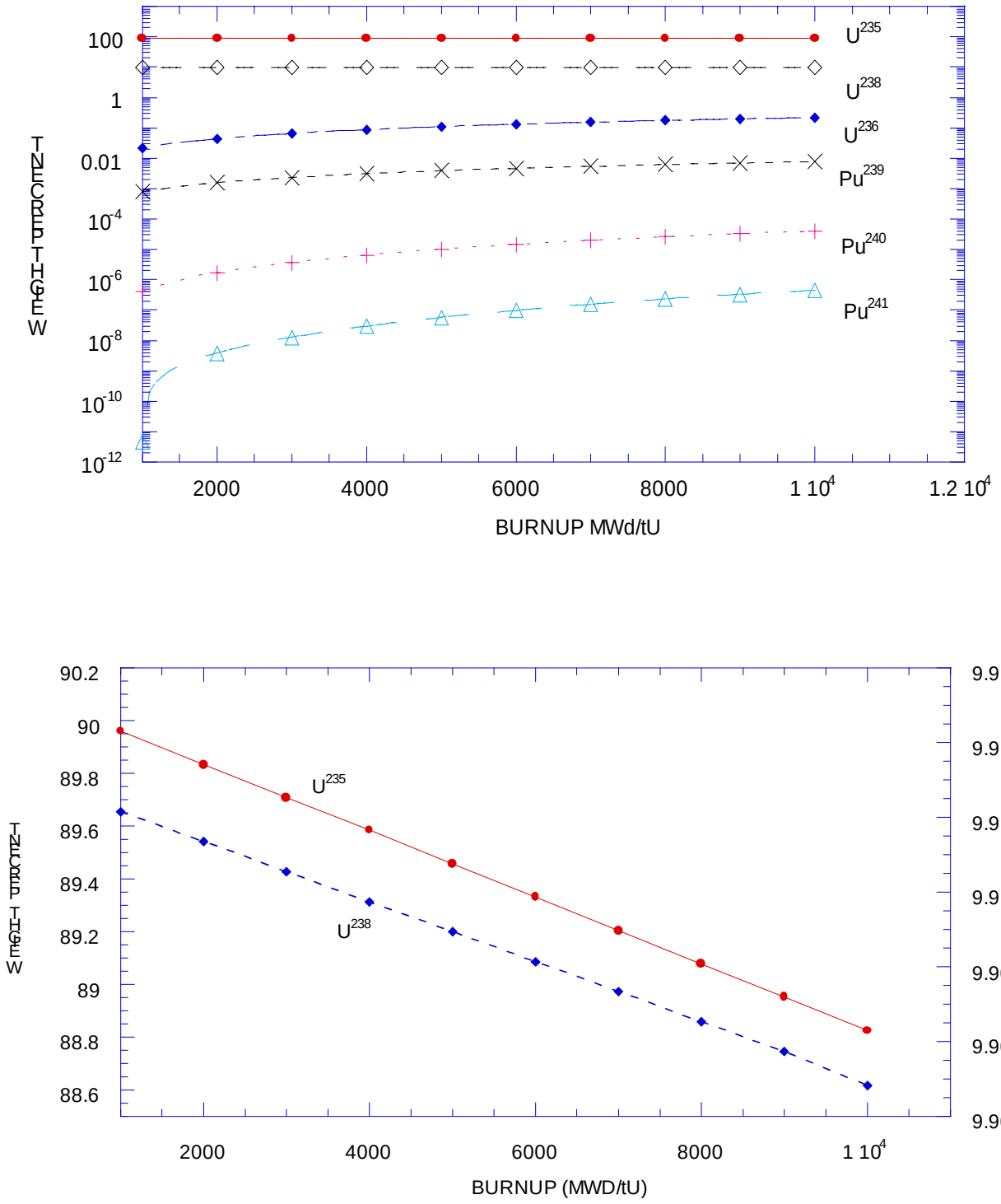
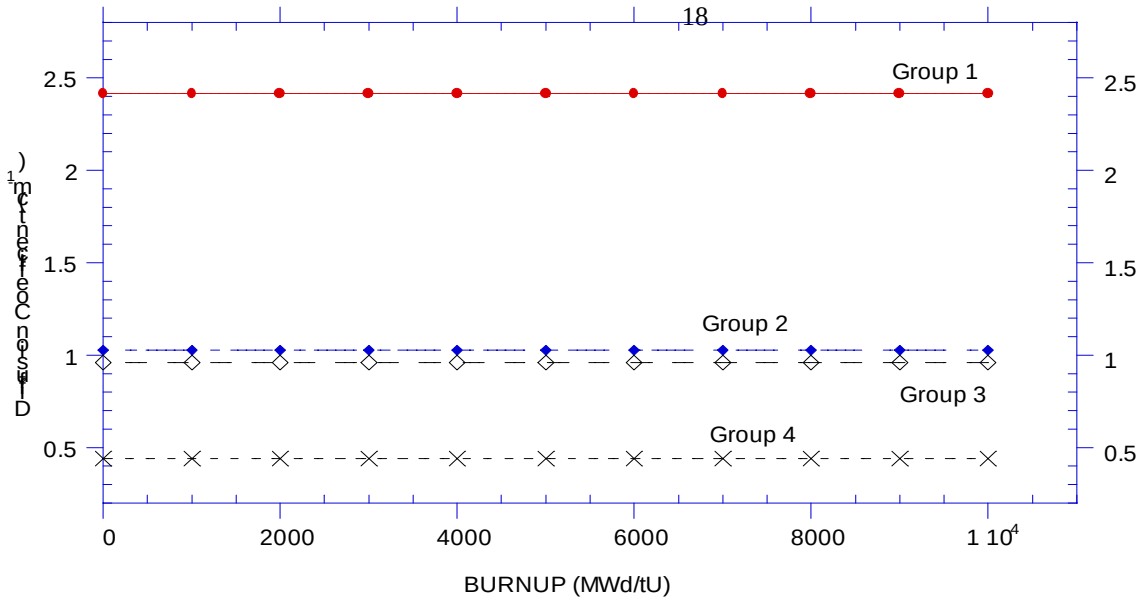
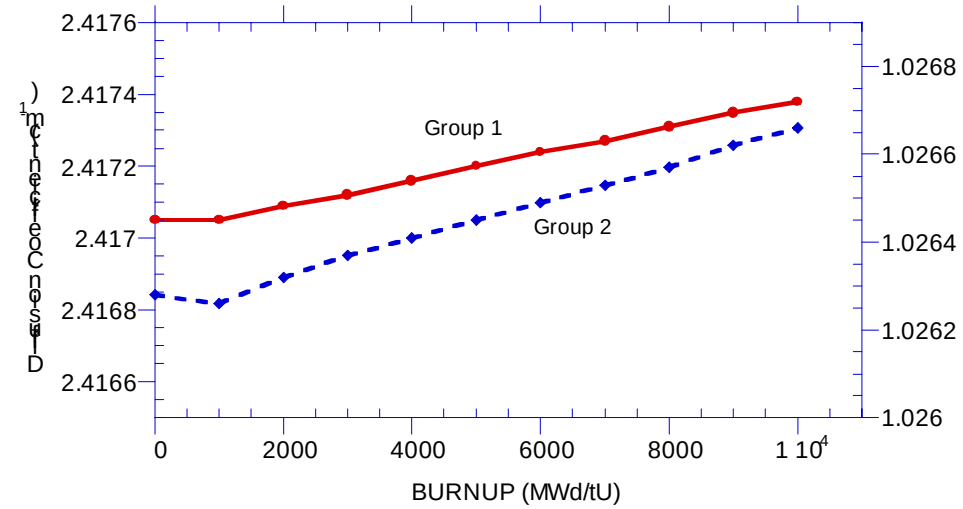


Fig. 8: Actinide Inventory: Weight Percent vrs. Fuel Burnup





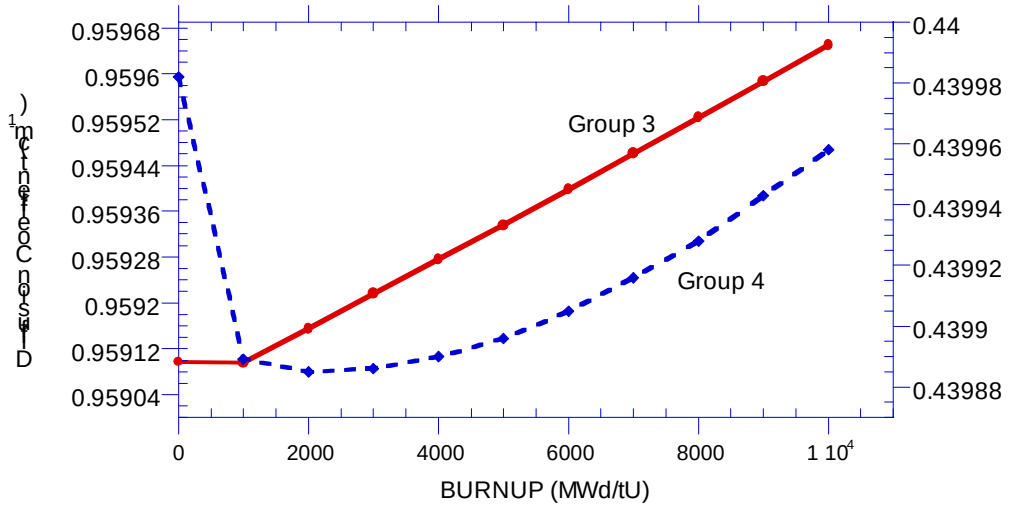


Fig. 9: Variation of Diffusion Coefficient with Fuel Burnup

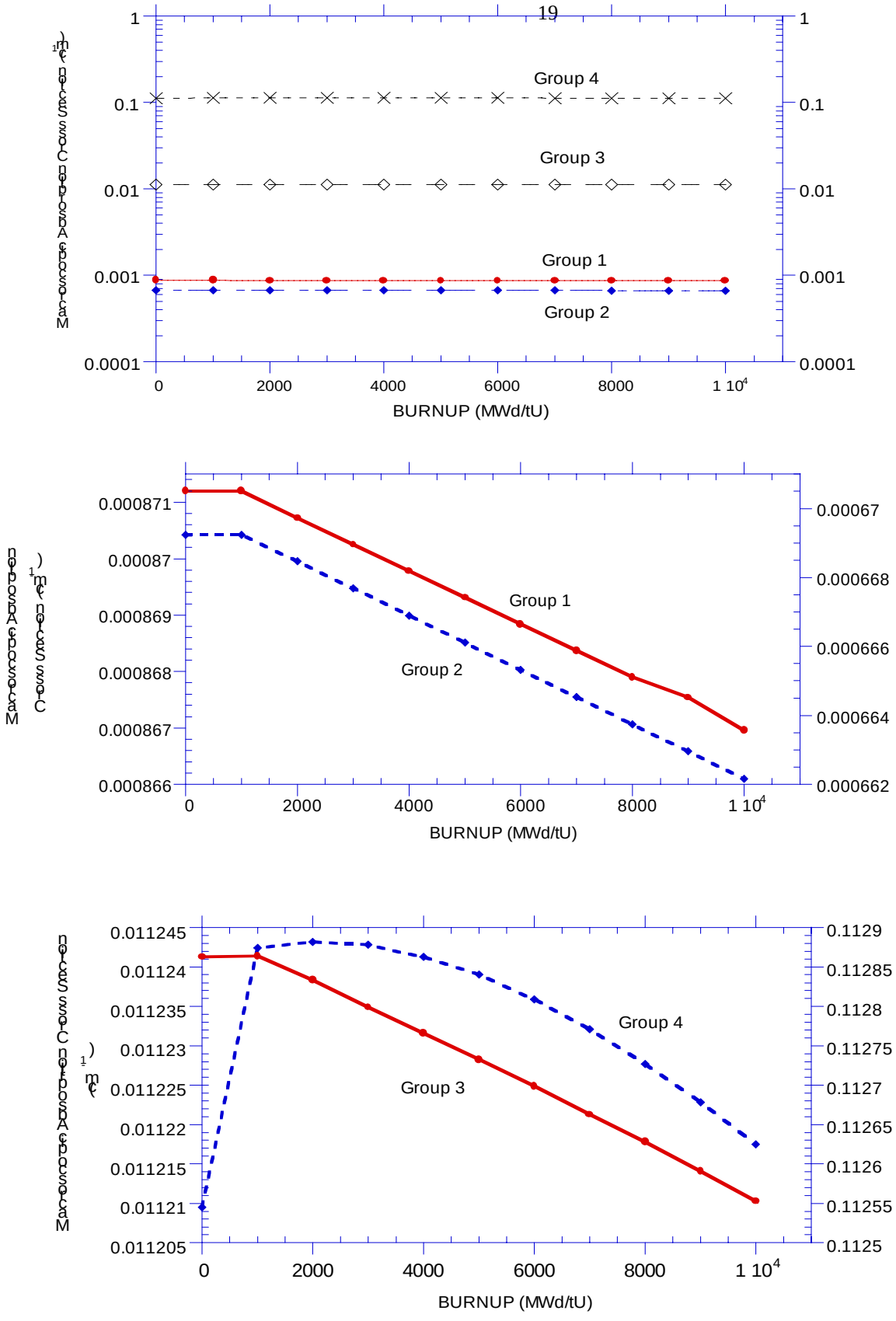


Fig. 10: Variation of Macroscopic Fission Cross Section with Burnup

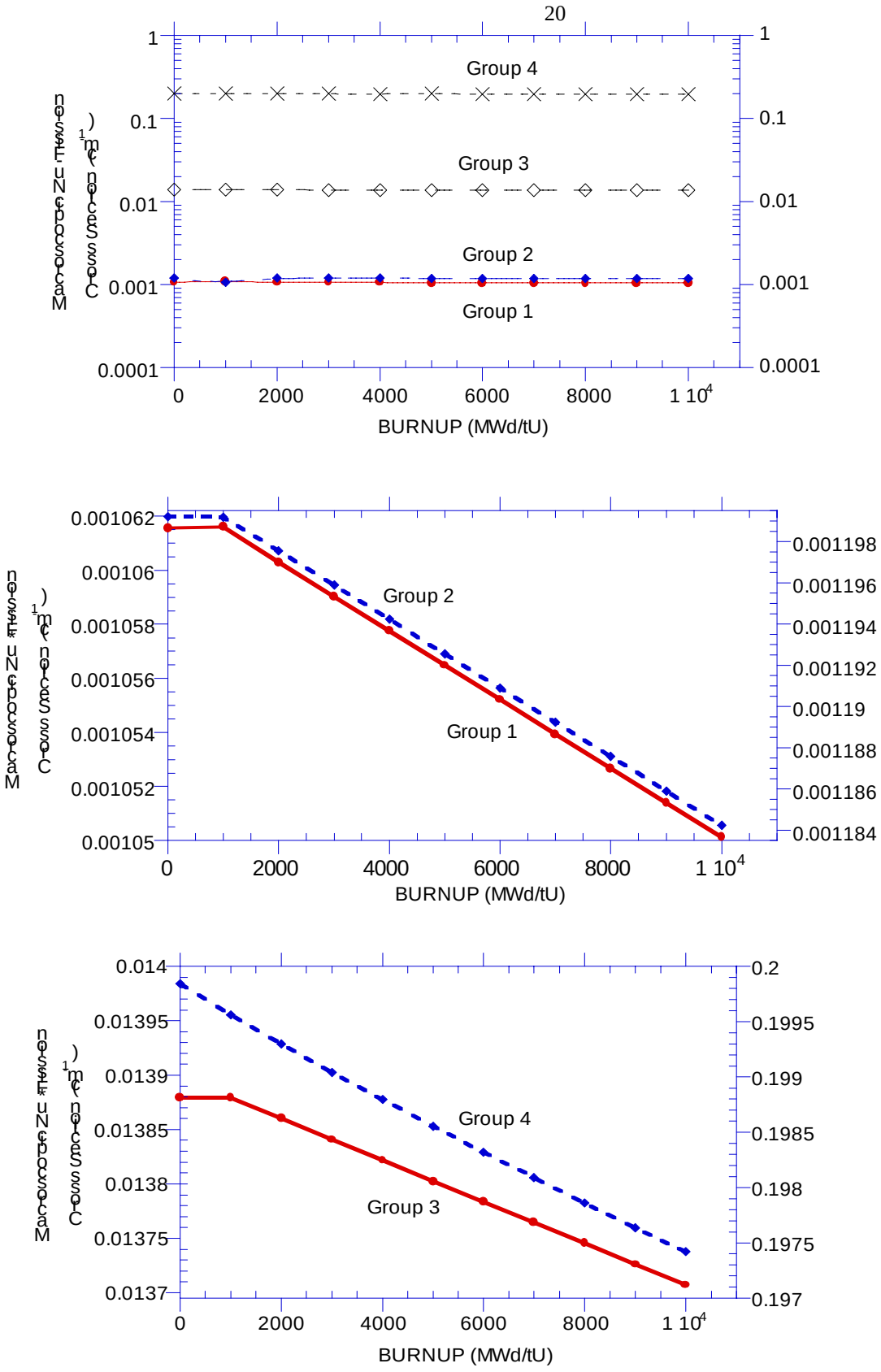


Fig. 11: Variation of Macroscopic Nu*Fission Cross Sections with Burnup

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